Corrigendum: On the calculation of x-ray scattering signals from pairwise radial distribution functions (2015 J. Phys. B: At. Mol. Opt. Phys. 48 244010)

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Corrigendum to: "On the Calculation of X-ray Scattering Signals from Pairwise Radial Distribution Functions"

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When we in Eq. (20) split up the scattering signal into contributions from solvent-solvent terms, solute-solvent (cross) terms, and solute-solute terms, each atom (type) belongs to either the solvent or the solute. Hence, the scattering signal contribution form the solute-solvent (cross) terms, Eq. (20*b*), should read:

$$S_{\mathrm{c}}(q) = 2\sum_{l}^{u}\sum_{m}^{v} f_l(q) f_m(q) \frac{N_l N_m}{V} 4\pi \int_0^{R_{\mathrm{box}}} r^2 [g_{l,m}(r) - 1] \frac{\sin(qr)}{qr} dr \qquad (20b)$$